Master 1 Statistique & Data Science, Ingénierie Mathématique

Apprentissage pour l'image Machine learning for image processing

Course II – Introduction to Artificial Neural Networks: Backpropagation

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Jeudi 21 mars 2024



Objectives

At the end of the course:

- Know what is a CNN (Convolutional Neural Network)
- Implement the training of a CNN for classification with Pytorch

For this session:

• Backpropagation to compute gradients in Neural Networks

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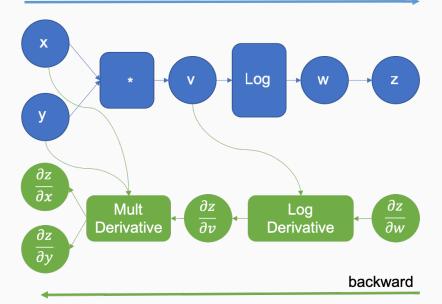
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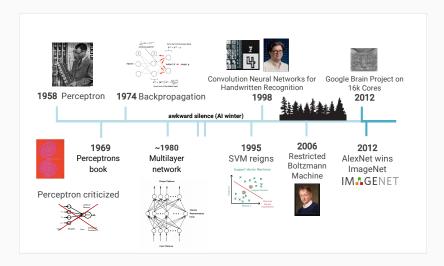
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forward



Timeline of (deep) learning

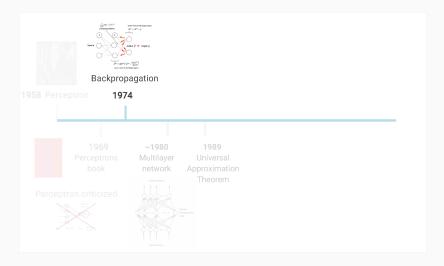


Backpropagation

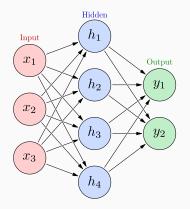


Machine learning - ANN - Backpropagation

Learning with backpropagation



Artificial neural network / Multilayer perceptron / NeuralNet



$$h_{2} = g_{1} \left(w_{21}^{1} x_{1} + w_{22}^{1} x_{2} + w_{23}^{1} x_{3} + b_{2}^{1} \right)$$

$$h_{3} = g_{1} \left(w_{31}^{1} x_{1} + w_{32}^{1} x_{2} + w_{33}^{1} x_{3} + b_{3}^{1} \right)$$

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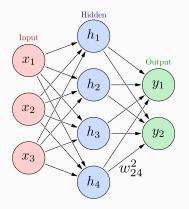
$$y_1 = g_2 \left(w_{11}^2 h_1 + w_{12}^2 h_2 + w_{13}^2 h_3 + w_{14}^2 h_4 + b_1^2 \right)$$

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 w_{ij}^k synaptic weight between previous node j and next node i at layer k.

 g_k are any activation function applied to each coefficient of its input vector.

Artificial neural network / Multilayer perceptron / NeuralNet



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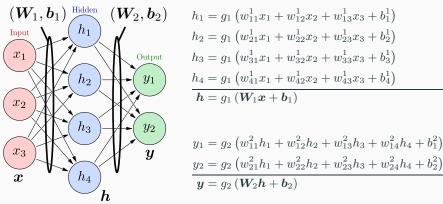
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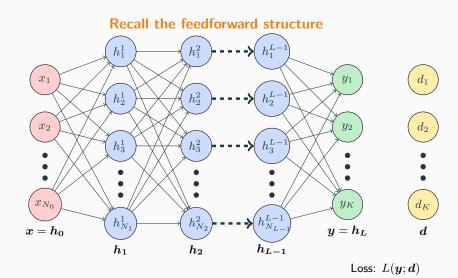
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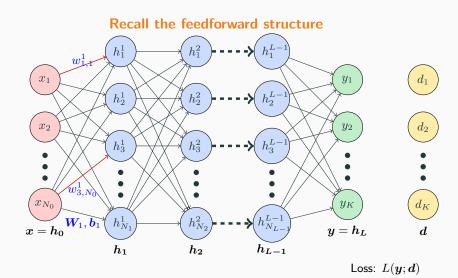
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The matrices W_k and biases b_k are learned from labeled training data.



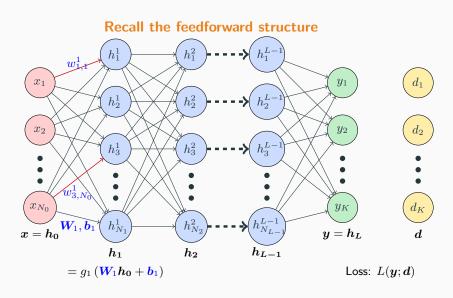
Hidden Layers

Output Layer



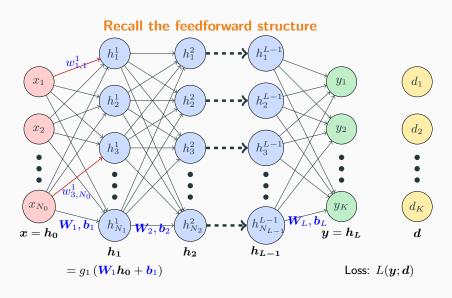
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- **Solution:** no closed-form solutions ⇒ use (stochastic) gradient descent.
- ullet $rac{\partial E(oldsymbol{W})}{\partial oldsymbol{W}_b}$ not really rigorous, we will use the notation

$$\nabla_{\boldsymbol{W}_k} E(\boldsymbol{W})$$
 and $\nabla_{\boldsymbol{b}_k} E(\boldsymbol{W})$.

Minimizing training loss

For multilayer neural networks $\boldsymbol{W} \mapsto E(\boldsymbol{W})$ is non-convex

 \Rightarrow No guarantee of convergence.

Even if convergence occurs, the solution depends on the initialization and the step size/learning rate γ .

Nevertheless, really good minima or saddle points are reached in practice by

$$\boldsymbol{W}^{t+1} \leftarrow \boldsymbol{W}^t - \gamma \nabla E(\boldsymbol{W}^t), \quad \gamma > 0$$

Gradient descent can be expressed coordinate by coordinate as:

$$w_{i,j}^{k,t+1} \leftarrow w_{i,j}^{k,t} - \gamma \frac{\partial E(\boldsymbol{W}^t)}{\partial w_{i,j}^k}$$

for all weights $w_{i,j}^k$ linking a node j to a node i in the next layer k.

$$\Rightarrow$$
 The algorithm to compute $\frac{\partial E(W)}{\partial w_{s,i}^k}$ for ANNs is called backpropagation.

- In practice we only use stochastic gradient descent with batch of training set.
- The complete loss is :

$$E(W) = \sum_{(\boldsymbol{x}^i, \boldsymbol{d}^i) \in \mathcal{T}} L(\boldsymbol{y}^i; \boldsymbol{d}^i)$$

ullet For some random small subset (e.g. batch) $\mathcal{S}\subset\mathcal{T}$, consider

$$E(\boldsymbol{W};\mathcal{S}) = \sum_{(\boldsymbol{x}^i, \boldsymbol{d}^i) \in \mathcal{S}} L(\boldsymbol{y}^i; \boldsymbol{d}^i)$$

Our goal is to compute the gradient

$$\nabla_{\boldsymbol{W}_k} E(\boldsymbol{W}; \mathcal{S}) = \sum_{(\boldsymbol{x}^i, \boldsymbol{d}^i) \in \mathcal{S}} \nabla_{\boldsymbol{W}_k} L(\boldsymbol{y}^i; \boldsymbol{d}^i).$$

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• Why is this relevant to minimize $E(\mathbf{W}) = E(\mathbf{W}; \mathcal{T})$?

Stochastic gradient descent: For some random small subset (e.g. batch)
 S ⊂ T, our goal is to compute the noisy gradient

$$\nabla_{\boldsymbol{W}_{k}}E(\boldsymbol{W};\mathcal{S}) = \sum_{(\boldsymbol{x}^{i}.\boldsymbol{d}^{i})\in\mathcal{S}} \nabla_{\boldsymbol{W}_{k}}L(\boldsymbol{y}^{i};\boldsymbol{d}^{i}).$$

• Unbiased approximation: As soon as ${\cal S}$ spans uniformly the whole training set ${\cal T}$,

$$\begin{split} \mathbb{E}_{\mathcal{S}}\left(\nabla_{\boldsymbol{W}_{k}}E(\boldsymbol{W};\mathcal{S})\right) &= \mathbb{E}_{\mathcal{S}}\left(\sum_{(\boldsymbol{x}^{i},\boldsymbol{d}^{i})\in\mathcal{S}}\nabla_{\boldsymbol{W}_{k}}L(\boldsymbol{y}^{i};\boldsymbol{d}^{i})\right) \\ &= \mathbb{E}_{\mathcal{S}}\left(\sum_{(\boldsymbol{x}^{i},\boldsymbol{d}^{i})\in\mathcal{T}}\mathbf{1}_{(\boldsymbol{x}^{i},\boldsymbol{d}^{i})\in\mathcal{S}}\nabla_{\boldsymbol{W}_{k}}L(\boldsymbol{y}^{i};\boldsymbol{d}^{i})\right) \\ &= \frac{|\mathcal{S}|}{|\mathcal{T}|}\sum_{(\boldsymbol{x}^{i},\boldsymbol{d}^{i})\in\mathcal{T}}\nabla_{\boldsymbol{W}_{k}}L(\boldsymbol{y}^{i};\boldsymbol{d}^{i}) = \frac{|\mathcal{S}|}{|\mathcal{T}|}\nabla_{\boldsymbol{W}_{k}}E(\boldsymbol{W}). \end{split}$$

• Conclusion: In expectation the noisy gradient is equal to the gradient using the whole training dataset (unbiased estimator).

Loss functions: Classical loss functions are:

For regression: $d^i \in \mathbb{R}^K$

Square error

$$E(\boldsymbol{W}) = \sum_{(\boldsymbol{x}^i, \boldsymbol{d}^i) \in \mathcal{T}} \frac{1}{2} \| \boldsymbol{y}^i - \boldsymbol{d}^i \|_2^2 = \sum_{(\boldsymbol{x}^i, \boldsymbol{d}^i) \in \mathcal{T}} \frac{1}{2} \sum_k (y_k^i - d_k^i)^2$$

For multi-class classification: $d^i \in \{1, \dots, K\}$, coded by $\boldsymbol{d}^i \in \{0, 1\}^K$,

Cross-entropy with softmax as the last layer

$$E(\boldsymbol{W}) = -\sum_{(\boldsymbol{x}^i, \boldsymbol{d}^i)} \sum_{k=1}^K d_k^i \log y_k^i \quad \text{with} \quad \boldsymbol{y}^i = f(\boldsymbol{x}^i; \boldsymbol{W}) = \text{softmax}(\boldsymbol{a}^i) \in (0, 1)^K.$$

ullet Cross-entropy with softmax included in loss (PyTorch convention): $y^i=a^i$ is the output of the last linear layer:

$$E(\boldsymbol{W}) = -\sum_{i=1}^{K} \left[a_{d^i} - \log \left(\sum_{k=1}^{K} \exp(a_k) \right) \right]$$
 with d^i the class of \boldsymbol{x}^i .

• The loss functions are of the form

$$E(\boldsymbol{W}) = \sum_{(\boldsymbol{x}^i, \boldsymbol{d}^i)} L(\boldsymbol{y}^i; \boldsymbol{d}^i)$$

By linearity,

$$\nabla E(\boldsymbol{W}) = \sum_{(\boldsymbol{x}^i, \boldsymbol{d}^i)} \nabla L(\boldsymbol{y}^i; \boldsymbol{d}^i)$$

- There the neural net output $m{y}^i = f(m{x}^i; m{W})$ is a function of the input data $m{x}^i$ and the neural weights $m{W}$.
- ullet We know the gradient of $L(oldsymbol{y}^i;oldsymbol{d}^i)$ with respect to the variable $oldsymbol{y}$
 - Regression/Square error:

$$L(\boldsymbol{y}; \boldsymbol{d}) = \frac{1}{2} \| \boldsymbol{y} - \boldsymbol{d} \|_2^2 \quad \Rightarrow \quad \nabla_{\boldsymbol{y}} L(\boldsymbol{y}; \boldsymbol{d}) = \boldsymbol{y} - \boldsymbol{d}$$

• Multi-class classification/cross-entropy:

$$L(\boldsymbol{y};\boldsymbol{d}) = -y_d + \log\left(\sum_{k=1}^K \exp(y_k)\right) \Rightarrow (\nabla_{\boldsymbol{y}} L(\boldsymbol{y};\boldsymbol{d}))_{\ell} = \operatorname{softmax}(\boldsymbol{y})_{\ell} - \delta_{\ell,d}.$$

ANN – Optimization

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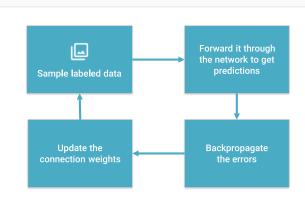
- There the neural net output $y^i = f(x^i; W)$ is a function of the input data x^i and the neural weights W.
- ullet We know the gradient of $L(oldsymbol{y}^i;oldsymbol{d}^i)$ with respect to the variable $oldsymbol{y}$
- We still need to compute

$$\nabla_{W_k} L(\boldsymbol{y}; \boldsymbol{d})$$
 and $\nabla_{\boldsymbol{b}_k} L(\boldsymbol{y}; \boldsymbol{d})$ for $k = 0, \dots, L$.

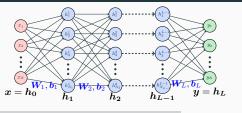
• For simplicity above we will use the notation E = L(y; d), that is considering only one point.

ANN - Learning

Training process



Learns by generating an error signal that measures the difference between the predictions of the network and the desired values and then using this error signal to change the weights (or parameters) so that predictions get more accurate.





 $\mathsf{Loss} \colon\thinspace E = L(\boldsymbol{y}; \boldsymbol{d})$

Forward pass

Initialization:

$$\boldsymbol{h}_0 = \boldsymbol{x}$$

for layer k=1 to L do

Linear unit:

$$\boldsymbol{a}_k = \boldsymbol{W}_k \boldsymbol{h}_{k-1} + \boldsymbol{b}_k$$

Componentwise non-linear activation:

$$\boldsymbol{h}_k = g_k(\boldsymbol{a}_k)$$

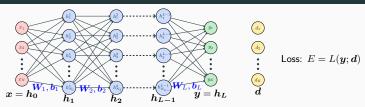
end

Output layer:

$$\boldsymbol{y} = \boldsymbol{h}_L$$

Compute loss:

$$E = L(\boldsymbol{y}; \boldsymbol{d})$$



Forward pass

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end

Output layer:

 $y = h_L$

Compute loss:

 $E = L(\boldsymbol{y}; \boldsymbol{d})$

Backward pass

Goal: Compute the gradient with respect to all parameters

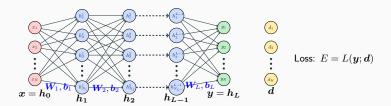
$$\frac{\partial E}{\partial w_{i,j}^k} = ?$$
 $\frac{\partial E}{\partial b_i^k} = ?$

for all

$$k \in \{1, \dots, L\},$$

$$i \in \{1, \ldots, N_k\}$$
,

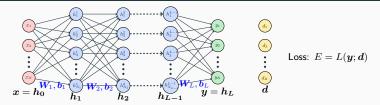
$$j \in \{1, \dots, N_{k-1}\}.$$



Going backward

• We know how to compute the loss function and its gradient:

$$\nabla_{\boldsymbol{h}_L} E = \nabla L(\boldsymbol{y}; \boldsymbol{d})$$



Gradient with respect to last linear unit output $oldsymbol{a}_L$

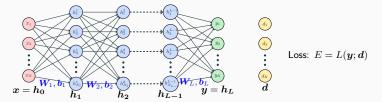
$$\boldsymbol{h}_L = q_L(\boldsymbol{a}_L)$$

That is for all $i \in \{1, \dots, N_L\}$, $h_i^L = g_L(a_i^L)$. By the chain rule,

$$\frac{\partial E}{\partial a_i^L} = \frac{\partial E}{\partial h_i^L} \frac{\partial h_i^L}{\partial a_i^L} = \left[\nabla_{\boldsymbol{h}_L} E \right]_i g_L'(a_i^L)$$

Vector formula:
$$\nabla_{\boldsymbol{a}_L} E = \nabla_{\boldsymbol{h}_L} E \odot g_L'(\boldsymbol{a}_L)$$

where \odot is the componentwise product between vectors, ie Hadamard product.



Gradient with respect to bias of last linear unit $oldsymbol{b}_L$

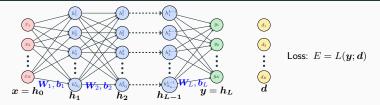
$$\boldsymbol{a}_L = \boldsymbol{W}_L \boldsymbol{h}_{L-1} + \boldsymbol{b}_L$$

That is for all
$$i \in \{1,\ldots,N_L\}$$
, $a_i^L = \sum_{j=1}^{N_{L-1}} w_{i,j}^L h_j^{L-1} + b_i^L$.

By the chain rule, for all $i \in \{1, \dots, N_L\}$,

$$\frac{\partial E}{\partial b_i^L} = \frac{\partial E}{\partial a_i^L} \underbrace{\frac{\partial a_i^L}{\partial b_i^L}}_{-1} = \frac{\partial E}{\partial a_i^L} = \left[\nabla_{\boldsymbol{a}_L} E\right]_i$$

Vector formula:
$$\nabla_{\boldsymbol{b}_L} E = \nabla_{\boldsymbol{a}_L} E$$



Gradient with respect to weights of last linear unit $oldsymbol{W}_L$

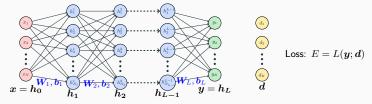
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, $a_i^L = \sum_{j=1}^{N_{L-1}} w_{i,j}^L h_j^{L-1} + b_i^L$.

By the chain rule, for all $i \in \{1,\dots,N_L\}$ and $j \in \{1,\dots,N_{L-1}\}$

$$\frac{\partial E}{\partial w_{i,j}^{L}} = \frac{\partial E}{\partial a_{i}^{L}} \underbrace{\frac{\partial a_{i}^{L}}{\partial w_{i,j}^{L-1}}}_{=h_{j}^{L-1}} = \frac{\partial E}{\partial a_{i}^{L}} h_{j}^{L-1} = \left[\nabla_{\boldsymbol{a}_{L}} E\right]_{i} \left[\boldsymbol{h}_{L-1}\right]_{j}$$

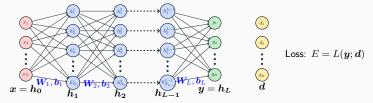
Matrix formula:
$$\nabla_{\boldsymbol{W}_L} E = \nabla_{\boldsymbol{a}_L} E \, \boldsymbol{h}_{L-1}^T$$



Gradients for last layer parameters

Given the gradient with respect to the output layer $\nabla_{\boldsymbol{h}_L} E$, so far we can compute:

- $\nabla_{\boldsymbol{a}_L} E = \nabla_{\boldsymbol{h}_L} E \odot g'_L(\boldsymbol{a}_L)$
- $\bullet \ \nabla_{\mathbf{b}_L} E = \nabla_{\mathbf{a}_L} E$
- $\bullet \ \nabla_{\boldsymbol{W}_{L}} E = \nabla_{\boldsymbol{a}_{L}} E \, \boldsymbol{h}_{L-1}^{T}$

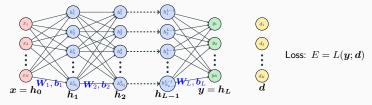


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How can we compute the gradients for the parameters of layer L-1?



Gradients for last layer parameters

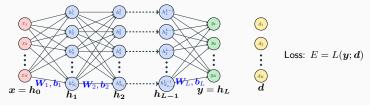
Given the gradient with respect to the output layer $\nabla_{h_L} E$, so far we can compute:

- $\nabla_{\boldsymbol{a}_L} E = \nabla_{\boldsymbol{h}_L} E \odot g_L'(\boldsymbol{a}_L)$
- $\nabla_{\mathbf{b}_T} E = \nabla_{\mathbf{a}_T} E$
- $\bullet \ \nabla_{\mathbf{W}_{L}} E = \nabla_{\mathbf{a}_{L}} E \, \mathbf{h}_{L-1}^{T}$

How can we compute the gradients for the parameters of layer L-1?

We need the expression of the gradient with respect to the last but one hidden layer $h_{L-1}...$ and then the same formulas apply!

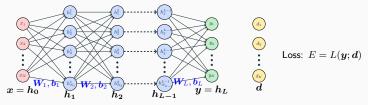
$$\nabla_{\boldsymbol{h}_{L-1}} E = ?$$



Gradient with respect to the last but one hidden layer $oldsymbol{h}_{L-1}$

Here, even to compute the scalar partial derivative $\frac{\partial E}{\partial h_j^{L-1}}$, we need to use differential calculus for multivariate functions since h_j^{L-1} appears in each component of a_L :

For all
$$i \in \{1,\dots,N_L\}$$
, $a_i^L = \sum_{j=1}^{N_{L-1}} w_{i,j}^L h_j^{L-1} + b_i^L$.



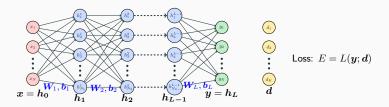
Gradient with respect to the last but one hidden layer $oldsymbol{h}_{L-1}$

Let us recall the derivative rule for composition with affine maps:

For
$$\varphi(x) = f(Ax + b)$$
 one has $\nabla \varphi(x) = A^T \nabla f(Ax + b)$.

Using the decomposition

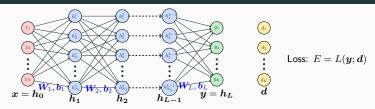
Vector formula:
$$\nabla_{\boldsymbol{h}_{L-1}} E = \boldsymbol{W}_L^T \nabla_{\boldsymbol{a}_L} E$$



We know $\nabla_{{m h}_{L-1}} E$ and :

•
$$h_{L-1} = g_{L-1}(a_{L-1}) \Rightarrow \nabla_{a_{L-1}} E = \nabla_{h_{L-1}} E \odot g'_{L-1}(a_{L-1})$$

- $a_{L-1} = W_{L-1}h_{L-2} + b_{L-1}$
- As before,
- $\bullet \ \nabla_{\boldsymbol{b}_{L-1}} E = \nabla_{\boldsymbol{a}_{L-1}} E$
- $\bullet \ \nabla_{\boldsymbol{W}_{L-1}} E = \nabla_{\boldsymbol{a}_{L-1}} E \boldsymbol{h}_{L-2}^T$



Forward pass

Initialization:

$$h_0 = x$$

for layer k=1 to L do

Linear unit:

$$\boldsymbol{a}_k = \boldsymbol{W}_k \boldsymbol{h}_{k-1} + \boldsymbol{b}_k$$

Componentwise non-linear activation:

$$\boldsymbol{h}_k = g_k(\boldsymbol{a}_k)$$

end

Output layer:

$$oldsymbol{y} = oldsymbol{h}_L$$

Compute loss:

$$E = L(\boldsymbol{y}; \boldsymbol{d})$$

Backward pass

Initialization: Gradient of output layer:

$$\nabla_{\boldsymbol{h}_L} E = \nabla L(\boldsymbol{y}; \boldsymbol{d})$$

for layer k = L to 1 do

Componentwise gain of error:

$$\delta_k = \nabla_{a_k} E = \nabla_{h_k} E \odot g_k'(a_k)$$

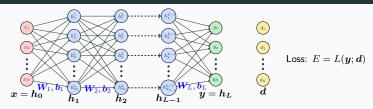
Gradient of layer bias:

$$\nabla_{\boldsymbol{b}_k} E = \boldsymbol{\delta}_k$$

Gradient of weights:

$$\nabla_{\mathbf{W}_k} E = \mathbf{\delta}_k \mathbf{h}_{k-1}^T$$

Gradient of previous hidden layer: $\nabla_{h_{k-1}} E = \boldsymbol{W}_k^T \boldsymbol{\delta}_k$



Forward pass

Initialization:

$$h_0 = x$$

for layer k=1 to L do

| Linear unit:

$$a_k = W_k h_{k-1} + b_k$$
 (stored)

Componentwise non-linear activation:

$$h_k = g_k(a_k)$$
 (stored)

end

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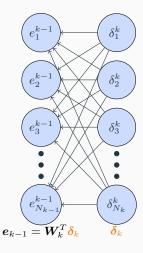
Gradient of layer bias:

$$\nabla_{oldsymbol{b}_k} E = oldsymbol{\delta}_k$$

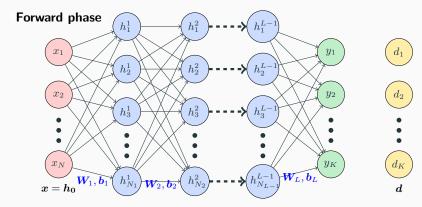
Gradient of weights:

$$\nabla_{\boldsymbol{W}_k} E = \boldsymbol{\delta}_k \boldsymbol{h}_{k-1}^T$$

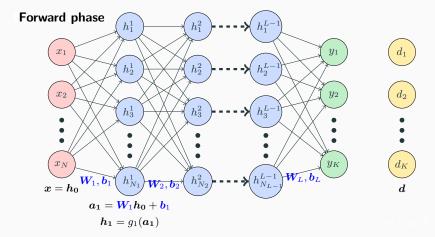
Gradient of previous hidden layer: $\nabla_{h_{k-1}} E = \boldsymbol{W}_k^T \boldsymbol{\delta}_k$



- Gradient of previous hidden layer: $e_{k-1} = \nabla_{h_{k-1}} E = W_k^T \delta_k$
- Multiplying by W_k^T corresponds to passing to the linear layer in reverse order.
- The error is backpropagated layer by layer to compute the gradient with respect to each layer parameters.



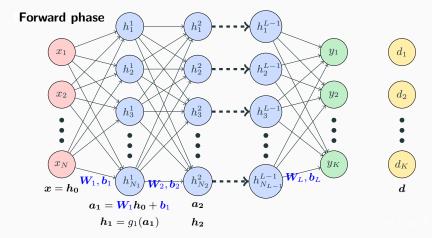
Input Layer Hidden Layers Output Layer Label



Input Layer

Hidden Layers

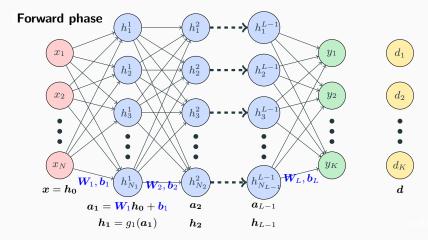
Output Layer



Input Layer

Hidden Layers

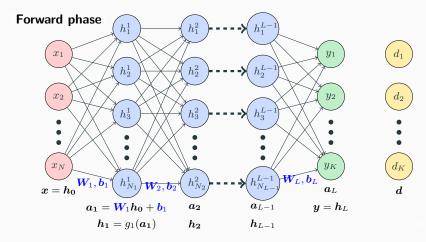
Output Layer



Input Layer

Hidden Layers

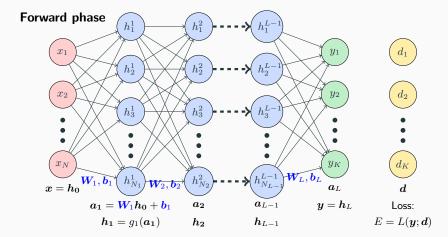
Output Layer



Input Layer

Hidden Layers

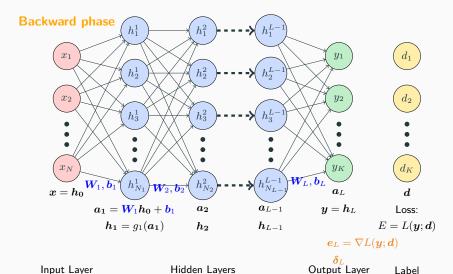
Output Layer

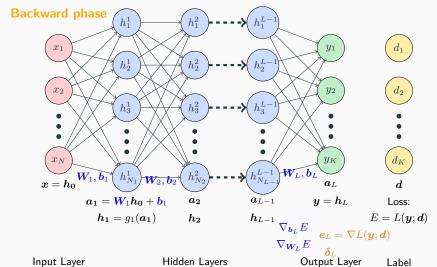


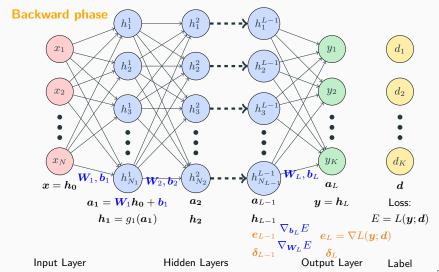
Input Layer

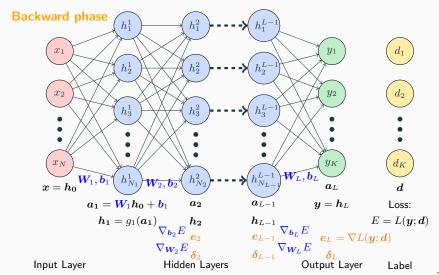
Hidden Layers

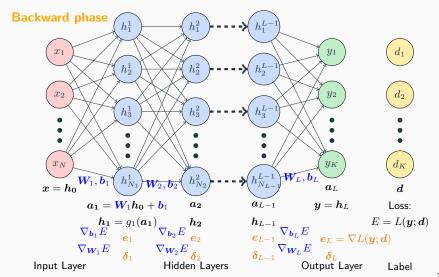
Output Layer

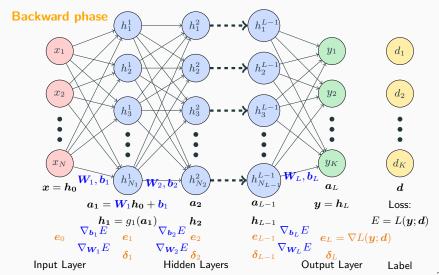












Error backpropagation in practice

Training loss:

$$E(\boldsymbol{W}) = \sum_{(\boldsymbol{x}^i, \boldsymbol{d}^i) \in \mathcal{T}} L(\boldsymbol{y}^i; \boldsymbol{d}^i)$$

- The backpropagation procedure computes $\nabla_{\mathbf{W}} L(\mathbf{y}^i; \mathbf{d}^i) = \nabla_{\mathbf{W}} L(f(\mathbf{x}^i; \mathbf{W}); \mathbf{d}^i).$
- ullet This has to be done for each data point $oldsymbol{x}^i \in \mathcal{T}.$
- By linearity, the final gradient $\nabla E(W)$ is the sum of all individual gradients $\nabla_W L(y^i; d^i)$.
- These gradients are summed sequentially (no need to store each individual gradients).
- In general we do not compute the exact gradient...

Error backpropagation in practice

Batch loss:

$$E(\boldsymbol{W}) \approx \sum_{(\boldsymbol{x}^i, \boldsymbol{d}^i) \in \mathcal{S}} L(\boldsymbol{y}^i; \boldsymbol{d}^i), \quad \text{with} \quad \mathcal{S} \subset \mathcal{T}$$

- ullet The backpropagation has to be done for each visited data point $x^i \in \mathcal{S}$ of the batch.
- ullet The gradient for each point x^i is added to the running gradient = current gradient estimation.
- Once the noisy estimated gradient is used as a gradient step, one needs to set the gradients to zero: See PyTorch torch.zero_grad() procedure.

Why is the backpropagation so efficient ?

- Avoid to re-do numerous computations
- No parameters need to be tuned
- Easy to implement
- This method can be seen as a Jacobian multiplication "in the right direction"

Some limitations:

- Memory consuming
- Backpropagation learning does not require normalization of input vectors; however, normalization could improve performance.

Questions?

Sources, images courtesy and acknowledgment

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V. Lepetit

L. Masuch